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by

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A Discontinuous Galerkin Discretization for the Mass Conservation Equation in the CE-QUAL-ICM Code

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1 Original discretization in the CE-QUAL-ICM code

The fundamental equation solved by the CE-QUAL-ICM code is the conservation of mass equation, written for each constituent convected by a flow:

$$\frac{\partial C}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(C v_i) - \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(D \frac{\partial C}{\partial x_i}) = s \tag{1}$$

where:

- C - concentration of a constituent $(gm\ m^{-3})$
- t, x_i - temporal and spatial coordinates $(x_1 = x,\ x_2 = y,\ x_3 = z)$
- $\boldsymbol{v} = [v_x, v_y, v_z]$ - fluid velocity $(m\ sec^{-1})$
- D - diffusion coefficient $(m^2 sec^{-1})$
- s - external loads, sources and sinks $(gm\ m^{-3} sec^{-1})$

The domain is a reservoir with the surface, the bottom and vertical boundaries perpendicular to x and y directions. The boundary conditions consist of the Neumann no-flow conditions on the surface and the bottom of the flow domain, and Dirichlet conditions on vertical boundaries.

In CE-QUAL-ICM the flow domain is divided into hexahedral control volumes (cells). It is assumed that cell faces are perpendicular to coordinate axes, but volumes do not necessarily form a regular structured mesh. Each cell is characterized by its volume and linear dimensions in each coordinate direction, and is limited by faces having specified area. Neither the cell volume nor the areas of cell faces can be, in general, computed using linear dimensions. It is assumed that the consistency of the whole specification of the mesh is guaranteed by programs supplying

CE-QUAL-ICM with geometry and flow data. The adopted model allows for more flexible treatment of the geometry of the flow domain (like changing elevation of the surface), but creates a certain arbitrariness in designing discretization formulas.

Time discretization is done using a splitting into two equations, the first for the horizontal flow and the second for the vertical flow. The horizontal step uses explicit time integration, while an implicit scheme leads to a system of linear equations in the vertical step.

In the actual computations the following values are assumed to be given at each time step: volumetric flows across faces, Q_k, and face areas, A_k; and diffusion coefficients on faces, D_k. Volumes, V_j, are specified initially and then updated using values of volumetric flows across faces (volumes of surface cells can be read directly from input files to allow for changing surface elevation). For each time step, sources, S_j, are computed by the program and the length Δt^n is determined based on CFL (Courant, Friedrichs and Lewy) number considerations. Concentrations within volumes are the primary unknowns of the discretization. Concentrations on faces, as well as gradients of concentrations on faces, are computed using the values within cells and the linear dimensions of cells.

2 Discontinuous Galerkin formulation

To derive a discontinuous Galerkin formulation [1, 2] for equation (1) the original CE-QUAL-ICM division of the computational domain Ω into hexahedral volumes V_j is assumed. The vertical boundaries of Ω form Dirichlet boundaries Γ_D, composed of

two parts: inflow Γ^-, and outflow Γ^+. Horizontal boundaries are Neumann no-flow boundaries. Boundaries between cells form the internal boundary, denoted by Γ_{int}. For an inter-cell boundary, Γ_{ef}, between two volumes V_e and V_f, jump and average operators are defined:

$$[v] = v|_{\partial V_e \times \Gamma_{ef}} - v|_{\partial V_f \times \Gamma_{ef}}$$

$$< v >= 0.5 * (v|_{\partial V_e \times \Gamma_{ef}} + v|_{\partial V_f \times \Gamma_{ef}})$$

The Baumann-Oden formulation of the discontinuous Galerkin method applied to equation (1) gives the following variational problem:

Find $C_h \in P_h^1$ such that for every test function $w \in P_h^1$the following holds:

$$\begin{aligned}
&\frac{d}{dt}\sum_j \int_{V_j} wC_h\, d\Omega = \sum_j \int_{V_j} ws\, d\Omega \\
&\quad + \sum_j \int_{V_j} \left(v_x \frac{\partial w}{\partial x} C_h + v_y \frac{\partial w}{\partial y} C_h + v_z \frac{\partial w}{\partial z} C_h \right) d\Omega \\
&\quad - \sum_j \int_{V_j} \left(D \frac{\partial w}{\partial x}\frac{\partial C_h}{\partial x} + D \frac{\partial w}{\partial y}\frac{\partial C_h}{\partial y} + D \frac{\partial w}{\partial z}\frac{\partial C_h}{\partial z} \right) d\Omega \\
&\quad + \int_{\Gamma_{int}} \left(-[v_n w]\bar{C}_h - D < \frac{\partial w}{\partial n} > [C_h] + D[w] < \frac{\partial C_h}{\partial n} > \right) d\Gamma \\
&\quad - \int_{\Gamma^-} v_n w C_D\, d\Gamma - \int_{\Gamma^+} v_n w C_h\, d\Gamma + \int_{\Gamma_D} \left(D \frac{\partial w}{\partial n}(C_D - C_h) + D w \frac{\partial C_h}{\partial n} \right) d\Gamma
\end{aligned} \tag{2}$$

where:

- P_h^1 - the space of cell-wise linear functions
- v_n - flow velocity normal to the flow face, $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$
- $\frac{\partial}{\partial n}$ - derivative normal to the flow face, $\frac{\partial}{\partial n} = \nabla \cdot \boldsymbol{n}$
- $\bar{C}$ - value of concentration on the upwind side of a face

- C_D - values specified on the vertical (Dirichlet) boundaries

Since cell faces are perpendicular to coordinate axes, the same splitting into horizontal and vertical flow as is used in the original CE-QUAL-ICM discretization can easily be performed. The integration for the horizontal flow problem extends only over vertical faces, while for the vertical flow only over horizontal faces. To keep in accordance with the discretization of CE-QUAL-ICM, the horizontal flow problem is discretized using an explicit method and the vertical flow problem using an implicit scheme.

The horizontal flow problem is solved first. Since the simplest explicit method, the forward Euler scheme, is unconditionally unstable for linear discontinuous Galerkin approximations [3], the second order Runge-Kutta algorithm is applied to the horizontal flow problem. This brings the advantage of the increased time accuracy to match the higher order accuracy of the discontinuous Galerkin approximation. The space discretization uses piecewise linear functions with the exact integration of terms appearing in the formulation (2).

2.1 Slope limiting

With the suitable time step restriction

$$\Delta t \leq 0.5 \min_j (\frac{l_x}{v_j}, \frac{l_y}{v_y})$$

(minimum is taken over both directions and all volumes) the time integration scheme is total variation diminishing (TVD) for the average values within cells. Still, there may appear oscillations for higher order linear degrees of freedom. To stabilize

these oscillations a minmod limiter has been implemented in the code [3]. The time integration scheme with slope limiting is total variation diminishing for time steps

$$\Delta t \leq \frac{1}{3} \min_j (\frac{l_x}{v_j}, \frac{l_y}{v_y})$$

and arbitrary Dirichlet boundary conditions.

3 Implementation

The discontinuous Galerkin approximation is implemented to minimize the changes introduced to the original CE-QUAL-ICM code. Only the parts of the code directly related to horizontal transport have been modified. This includes initialization of variables, calculations of auxiliary geometric quantities and time step length computation. Each modification done to the original CE-QUAL-ICM code is explicitly delimited by the lines

```
CDGbegin KB - added Discontinuous Galerkin transport scheme
```

and

```
CDGend KB - added Discontinuous Galerkin transport scheme
```

New arrays for additional degrees of freedom `CX` and `CY`, as well as volume updates `DTCX` and `DTCY`, are declared in the include file *wqm_com.inc*. It was assumed that memory savings are less important than code efficiency, and several auxiliary arrays have been declared in the *wqminit_com.inc* file. In the same file there are logical variables `DG` and `DGSL` for two types of discontinuous Galerkin discretization, the first without and the second with slope limiting. All variables in the included files are made global through definitions of appropriate common blocks.

At the current stage the discontinuous Galerkin approximation is implemented only for the horizontal flow problem. The flow of computations is controlled by the values of variables `DG` and `DGSL`. If one of them is `TRUE` the code updates the unknown degrees of freedom using the scheme described above. The time-step length chosen for the discontinuous Galerkin approximation is half of that used for the QUICKEST algorithm. If the `DGSL` option is specified, slope limiting is applied after two sweeps of the Runge-Kutta algorithm.

It is assumed that the solution to the vertical problem is done by the original CE-QUAL-ICM algorithm using the average values of concentrations within cells.

4 Running CE-QUAL-ICM with the discontinuous Galerkin approximation

The only change in the input file necessary to run the CE-QUAL-ICM code with the discontinuous Galerkin approximation is the specification of the approximation type `DG` or `DGSL` instead of the existing `UPWIND` or `QUICKEST` types. The `DG` algorithm provides more accurate but less stable approximations, and the `DGSL` algorithm eliminates unwanted oscillations in the solution. If the chosen time-step limit turns out to be insufficient to guarantee stability, changing the parameter `DLTFTN` to 0.6 should make the scheme stable, even for difficult boundary conditions.

References

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